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**SENSITIVITY ANALYSIS OF COMPLEX COUPLED SYSTEMS
TO SECOND AND HIGHER ORDER DERIVATIVES**

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Introduction

In design of engineering systems, the "what if" questions often arise such as: what will be the change of the aircraft payload, if the wing aspect ratio is incremented by 10 % ? Answers to such questions are commonly sought by incrementing the pertinent variable, and reevaluating the major disciplinary analyses involved. These analyses are contributed by engineering disciplines that are, usually, coupled, as are the aerodynamics, structures, and performance in the context of the question above.

The "what if" questions may be answered exactly without using the "increment-and-reevaluate" approach and without finite differencing of the system analysis, by using a method introduced in ref.1 for calculating the first derivatives of behavior of coupled systems with respect to design variables. The method called the system sensitivity analysis has been shown applied in formal optimization that used the derivatives to guide search in multidimensional design space, e.g., ref.2 and 3. Obviously, if the problem is strongly nonlinear, the efficiency of such search will improve if second and, possibly, higher order derivatives are available to the search algorithm. A need for the second derivatives to enhance the method of ref.1 applied in such problems is discussed in ref.4.

This note extends the algorithm of ref.1 to include the derivatives of the second and higher orders, again, without finite differencing of the system analysis. It achieves that by recursive application of the same implicit function theorem that underlies ref.1. As a supplement to ref.1, the note is not self-contained, it references equations in ref.1 (such references are shown as "eq.no/ref.1") and requires that reference as a prerequisite.

First Order Sensitivity Analysis

Sensitivity problem stated in ref.1 calls for calculation of the derivatives of a vector Y solving the governing equations, eq.1/ref.1, with respect to a design variable X_k . The algorithm developed in ref.1 yields the derivative of Y as a solution vector Z of the sensitivity equations which are linear, simultaneous, algebraic equations of the form

$$1 \quad A Z = R$$

In ref.1, the terms in the above equation are defined by two equivalent sets of equations: either eq.4/ref.1 (based on the residuals and called the Global Sensitivity Equations 1, GSE1) or eq.8/ref.1 (based on the output/input partial sensitivity derivatives and called the Global Sensitivity Equations 2, GSE2). The contents of the matrix of

coefficients A and the right hand side (RHS) vector R are different for the above two alternative formulations but the solution vector Z is the same and represents the derivative of Y with respect to the k-th element of the vector of design variables X. It has the meaning of the total derivative because it reflects both the direct and indirect influences of X_k on Y.

Sensitivity Analysis of Second and Higher Orders

Generalization of the above first order sensitivity analysis to the higher orders is straightforward by taking advantage of the linearity of eq.1 above. Although most of the linear algebra texts ignore the matter, algorithms for sensitivity analysis of the linear algebraic equations solution have been developed in structural sensitivity analysis. They stem from the same implicit function theorem that was the basis for ref.1, e.g., ref.5 and 6, and they extend to the second order derivatives, e.g., ref.7 and 8. The pattern established in these algorithms will be adapted to solve the problem at hand.

A compact notation for the derivatives will be used in the remainder of the note

$$3 \quad (\)_{qk1m\dots} = \partial q(\) / \partial X_k \partial X_1 \partial X_m \dots$$

where any subscript may be repeated as required to form a high order, mixed derivative with respect to any combination of variables X.

In the above notation, the correspondence of eq.1 above to eq.4/ref.1 and eq.8/ref.1 makes the derivatives of Z with respect to X equivalent to the derivatives of Y with respect to X, as follows (Z is already the first derivative of Y):

$$\begin{aligned} 4 \quad Z^0 &= Y^1_k \\ Z^{11} &= Y^{2}_{k1} \\ Z^{21m} &= Y^{3}_{k1m} \\ &\dots\dots\dots \\ Z^{N1m\dots} &= Y^{N+1}_{k1m\dots} \end{aligned}$$

Repeated differentiation of eq.1 yields the derivatives of Z according to a regular pattern, shown below up to the fourth derivative

$$\begin{aligned} 5 \quad A Z^{11} &= R^{11} - A^{11} Z^0; \\ 6 \quad A Z^{21m} &= R^{21m} - A^{1m} Z^{11} - D^{1m}(A^{11} Z^0); \\ 7 \quad A Z^{31mn} &= R^{31mn} - A^{1n} Z^{21m} - D^{1n}(A^{1m} Z^{11}) - D^{2mn}(A^{11} Z^0); \\ 8 \quad A Z^{41mnp} &= R^{41mnp} - A^{1p} Z^{31mn} - D^{1p}(A^{1n} Z^{21m}) - D^{2np}(A^{1m} Z^{11}) \\ &\quad - D^{3mnp}(A^{11} Z^0); \\ &\dots\dots\dots \\ &\text{etc.} \end{aligned}$$

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where $D_{q1mn}()$ is a shorthand for the q -th mixed derivative of the product of the pair of functions named in the parentheses, obtained by the usual rules of the product differentiation. Here, again, any subscript may be repeated. Once the derivatives of Z are obtained, the derivatives of Y are available from eq.4.

The computational cost of a full set of mixed, derivatives of the N -th order obtained by means of the above algorithm escalates rapidly with the value of N . Firstly, because the number of derivatives in a complete set is proportional to the number of the design variables d raised to the N -th power, and, secondly, because the eq.5-8 are recursive. Inspection of the A terms and the D terms reveals that in the calculation of a mixed derivative of the N -th order referencing a particular variable, the recursivity requires derivatives of the orders $N-1$ and lower with respect to the same variable as prerequisites. For example, to solve eq.8 for Z^{41mnp} , the prerequisites are the derivatives Z^{31mn} , Z^{31mp} , Z^{31np} , and Z^{3mnp} .

On the other hand, due to the recursivity all the eq.5-8 share the same matrix A so that matrix needs to be factored only once and reused when the equations are solved one after another. Each solution requires, then, only a backsubstitution of its RHS over the factored A - a task ideally suited to the modern vector and parallel processor computers.

Special Case of Single Variable

The recursivity becomes also an advantage if there is only one variable with respect to which the derivatives are to be taken. It is the case of interest because it occurs in searching design space along a line defined by a search direction S - an operation that is a part of many optimization algorithms. Accurate extrapolation based on higher order derivatives may reduce the need for costly repetitions of the system analysis in that operation by widening the move limits. Assuming that the direction vector S has already been generated, all the variables X_k become linked to the step length h through S so that

$$9 \quad X_{\text{new}} = X_{\text{old}} + h S$$

This relation enables one to substitute X with h in eq.1/ref.1, and by chain differentiation to replace the right hand sides of eq.4/ref.1 and eq.8/ref.1 with

$$10 \quad \text{RHS}(h) = \sum_{k=1}^d S_k \text{RHS}(X_k)$$

where $\text{RHS}(h)$ is the right hand side vector reflecting the presence of only a single variable h , $\text{RHS}(X_k)$ refers to the RHS in eq.4/ref.1 or 8/ref.1 related to a variable X_k , and S_k is the k -th element of S .

With the problem reduced to a single variable h , the variable identification subscripts are no longer needed, and R in eq.1 may be replaced with

$$11 \quad R = \text{RHS}(h)$$

from eq.10 to transform the pattern of equations, eq.5 through eq.8, to

$$\begin{aligned}
 12 \quad & A Z^1 = R^1 - A^1 Z^0; \\
 13 \quad & A Z^2 = R^2 - A^1 Z^1 - D^1(A^1 Z^0); \\
 14 \quad & A Z^3 = R^3 - A^1 Z^2 - D^1(A^1 Z^1) - D^2(A^1 Z^0); \\
 15 \quad & A Z^4 = R^4 - A^1 Z^3 - D^1(A^1 Z^2) - D^2(A^1 Z^1) - D^3(A^1 Z^0); \\
 & \dots\dots\dots \\
 16 \quad & A Z^N = R^N - A^1 Z^{N-1} - \sum_{s=1}^{N-1} D^s(A^1 Z^{N-1-s-1})
 \end{aligned}$$

By the Leibniz's rule (e.g., ref.9) the D-terms may be written as

$$17 \quad D^s(A^1 Z^{N-1-s-1}) = \sum_{q=0}^s (C^s_q A^{1+s-q} Z^{N-s-1+q})$$

where C^s_q are the binomial coefficients

$$18 \quad C^s_q = s! / (q! (s-q)!); C^s_s = C^s_0 = 1; C^s_1 = s;$$

also obtainable from the Pascal's triangle (ref.9).

Structural Sensitivity Analysis: A Special Case of A Linear System

Another special case arises when the governing equations, eq.1/ref.1, are linear algebraic simultaneous equations. For an instance, consider the load-deflection equations in the displacement method of structural analysis

$$19 \quad K W = P$$

where the stiffness matrix K and the load vector P may be functions of design variables X , so that the vector of displacements becomes an implicit function of X . If one substitutes the terms in eq.1 as follows

$$20 \quad A = K; Z = \partial W / \partial X_k; R = \partial P / \partial X_k - \partial K / \partial X_k W;$$

then eq.4 through eq.18 formulate the structural sensitivity analysis through the N -th order derivatives (including the case of derivatives taken in a direction S in the design space).

Since K is a linear function for a broad class of design variables (e.g., the wall thickness in a membrane structure, or the moment of inertia of a beam cross-section), the patterns of eq.5 - 8 and 12 - 16 simplify drastically because the terms comprising the second and higher derivatives of K vanish. When one wishes to compute derivatives for only a subset of W , then further simplifications and computational cost savings are available by the use of an alternative known as the adjoint variable method (ref.6 and 7 discuss that method including the second derivative applications) that is, however, beyond the scope of this note.

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